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ABSTRACT

Research in the area of multivariate outliers is reviewed, emphasizing the problems associated with definition and identification. Treatment of the problem can be traced to 1777 and the work of D. Bernoulli. Most of the many procedures developed for identifying outliers proceed sequentially starting with the most aberrant observation, or proceed without consideration of the influence that an outlier may have on the focus of the analysis. If an outlier does not influence the outcome, there may be no reason to be concerned with it. A major problem in identifying outliers has been the lack of agreement on an operational definition of "outlier," even though most definitions refer to the outlier as being extreme in some manner. Researchers must reach a consensus on the definition in order to proceed in perfecting identification procedures. Once an outlier is identified, its treatment is contingent upon the type of data being studied. Outliers may be of such importance as to be the main focus of some types of study. A list of 64 references is included. (SLD)

Review of the Literature: Multivariate Outliers

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Introduction

Research on the problem of multivariate outliers has focused on several areas: definition, identification and accommodation (Beckman & Cook, 1983). Accommodation includes both rejection and weighting of the outlying observations. This review examines the research in the area of multivariate outliers while emphasizing the problems associated with definition and identification.

Historical Review of the Problem

Treatment of the problem of outliers in statistical analysis can be traced back to the work of Bernoulli in 1777. Bernoulli stated that not all observations have the same weight or error, yet he questioned the practice of deleting these aberrant observations completely. Chauvenet proposed a method for detection of "gross errors" as early as 1850 (Dixon, 1951, p. 68). Throughout the nineteenth century work was done on the identification and rejection of outliers in the univariate case by Peirce, Gould, Glaisher, Edgeworth, Stone, and Newcomb (Stone, 1873; Newcomb, 1886; Beckman & Cook, 1983). Glaisher and Newcomb used a weighted least squares method. As of 1950 Dixon wrote that there had been no success in the development of a criterion for discovery of outliers by means of a general statistical theory.

Definitions of Outlier

Many of the researchers who have dealt with the problem of outliers have based their work on a subjective definition of an outlier. Dixon (1950) saw an outlier as a value which is "dubious in the eyes of the analyst" (p. 488). Grubbs (1969) said an outlier "appears to deviate markedly from other members of the sample" (p. 1), and Elashoff and Elashoff

(1970) stated it is an observation which is "extreme in some sense" (p. 4). Many other researchers have used the same basic definition (Pascale & Lovas, 1976; Barnett, 1978; Barnett & Lewis, 1978; Robertson, 1987; & Rasmussen, 1988).

By the mid 1970's the definition of an outlier was becoming more complex. Guttman (1973a) saw an outlier as a spurious observation which did not come from a $N(\mu,\sigma^2)$ population. Gentleman and Wilk (1975b) pointed out that an outlier could be an outlier only "relative to some prespecified model or theory..." (p. 389), an idea supported by Gentle (in David, 1978). At this same time Rohlf (1975) referred to "points which are not internal to the cloud of points" (p. 93) as potential outliers. Along the same lines, Hawkins (1980) defined multivariate outliers as "values with high probabilities of occurring where the probability density of the true distribution is low, remote from the main body of data" (p. 104). Campbell (1980) categorized multivariate outliers as values which "fail to maintain the pattern of relationships between the variables evident in the majority of the observations" (p.231); Hoaglin, Mosteller, and Tukey (1983) offered a similar definition when they talked of "different underlying behavior for certain values as compared with that for the bulk of the data" (p. 39).

In the 1980's some authors began to use statistical properties to describe outliers. Huber (1981) stated that a large h_i is a "warning signal" (p. 161) for an outlier. Anscombe and Tukey (quoted in Schwager & Margolin, 1982, p. 943) referred to outliers as having large residuals, a definition which was supported by Portnoy (1988) when he referred to an outlier an any observation "whose residual from some linear model is unusually large compared to most other residuals from this model" (p. 2). Portnoy also called an

observation an outlier if it is more than five standard deviations from the model. In 1983 Beckman and Cook (1983) stated that the definition of an outlier was still "vague", but that with the "emphasis on modeling in recent years, 'outlier' now seems to be used ... to indicate any observation that does not come from the target population" (p. 121). Barnett (in discussion of Beckman & Cook, 1983) put the idea into perspective when he said, "What is vital is not whether an arbitrary observation x_i is way out in the tails of F, but whether (for example) the largest observation $x_{(n)}$ is unreasonably large as an observation of $X_{(n)}$ under F" (p. 150). Comrey (1985) seemed to regress from an operational definition when he said that outliers are "incorrect measurements that contaminate data" (p. 273).

By the late 1980's researchers were interested in outliers in multiple regression. Douzenis and Rakow (1987) defined an outlier as a value which is "extremely deviant from the regression line" (p. 1). Chatterjee and Hadi (1988) were referring to linear regression when they defined an outlier as an "observation for which the studentized residual (r_i or r_i^*) is large in magnitude compared to other observations in the data set" (pp. 94-95). They also differentiated between high leverage points and influential points. High leverage points are "those for which the input vector x_i is, in some sense far from the rest of the data" as defined by Hocking and Pendleton (quoted in Chatterjee & Hadi, 1988, p. 95); influential points are defined as "those observations that, individually or collectively, excessively influence the fitted regression equation as compared to other observations in the data set" (Chatterjee & Hadi, 1988, p. 95). Taylor (1989) said that the above definition of an "influential point" was vague, although he described outliers as observations which have an "undue influence on the inferences obtained from statistical models" (p. 2), and he went on to state a concern for a

definition of "influence". Simonoff (1989) defined outliers as influential points or leverage points.

Booth, Alam, Ahkam, and Osyk (1989) pointed out the difficulty of defining a multivariate outlier when they referred to a statistical outlier as a nonrepresentative observation whose "position may not be extreme enough on the basis of a single variable to demonstrate its outlying characteristics. However, the combined effects of several variables could be substantial enough to justify categorizing" (p. 321) it as an outlier.

Rousseeuw and von Zomeren (1990) stated that outliers are an "empirical reality but their exact definition is as elusive as the exact definition of a cluster" (p. 650). They suggested that outliers are "observations that deviate from the model suggested by the majority of the point cloud, where the central model is a multivariate normal" (Rousseeuw and von Zomeren, 1990, p. 651). This idea goes back as far as 1975 with Rohlf.

Outlier Identification

Identification of outliers is critical because "many of the standard multivariate methods are derived under the assumption of normality and the presence of outliers will strongly affect inferences made from normal-based procedures" (Schwager & Margolin, 1982, p. 943).

Some of the procedures for identifying multivariate outliers have been adapted from the univariate methods developed during the twentieth century. These procedures include the generalized studentized residual (Siotani, 1959), the ratio of generalized distance with k outlying observations deleted to generalized distance with all observations (Wilks, 1963), the W statistic for normality (Shapiro & Wilk, 1965), the examination of the residuals of each

variable regressed on the other variables (Cox, 1968; Guttman, 1973a), the gap test (Rohlf, 1975), and a Bayesian technique (Guttman, 1973b). Devlin, Gnanadesikan, and Kettenring (1975) proposed the use of the sample product-moment correlation coefficient or of scatter plots "augmented by influence function contours" (p. 533). Brown (1975) suggested an outlier test which analyzes patterns among the signs of the residuals; the presence of outliers would disturb the balance of plus and minus signs.

Many procedures involve the use of residuals. Prescott (1975) proposed a statistic using residuals standardized by individual standard deviations. Cook (1977) advocated using plots of residuals or examining the standardized residuals or studentized residuals. The studentized residual is a measure of the degree to which an observation is an outlier. Cook's *D* is considered a measure of the overall impact any single point has on the least squares solution. It is a combined measure of the lack of fit and of the distance in factor space according to Wood (1983), but it suffers from masking because it is a sequential process. Cook (1986) recommended using D_i as a "basis for detecting cases that should be inspected for gross errors" (p. 135). Gentle (in David, 1978) suggested that, if there is only one outlier, the maximum absolute studentized residual, R_n, can be used to identify the outlier; however, in the case of multiple outliers, the effectiveness of *R* suffers. Gentle recommended several procedures for use in the case of multiple outliers: Andrews' idea to project the residual vector onto hyperplanes generated by all combinations of pairs of columns, Mickey's forward selection process, and Gentleman and Wilk's regression using all subsets of the data with *k* observations removed.

Barnett and Lewis (1978) categorized the available procedures into six types: the excess spread statistic, the range spread statistic, the deviation spread statistic, the sums of squares statistic, the high-order moment statistic, and the extreme location statistic. The first type is represented by Dixon's (1951) ratio involving values; the second is a ratio of range to standard deviation proposed by David, Hartley, and Pearson in 1954; the third and fourth procedures were presented by Grubbs in 1950. The fifth type, high-order moment statistics, was done by Ferguson in 1961, Shapiro and Wilk (1965), and Shapiro, Wilk, and Chen (1968). The final type is presented by Epstein in 1960 and Likěs (1966).

Other multivariate procedures which are not extensions of univariate methods have been developed in the last twenty years. Andrews (1972) suggested a plotting technique using a function of the data points. Hawkins (1974) recommended using principal components.

Hoaglin and Welsch (1978) proposed the use of the hat matrix, since the information therein can reveal outliers. The diagonal elements can be interpreted as the amount of leverage or influence exerted on the predicted y value by y_i. Huber (1975) agrees that the h_i shows the researcher the points where the value of y has a large impact on the fit. Hoaglin and Welsch (1978) suggested using the hat matrix with the studentized residual and "tag(ging) as exceptional any point for which h or r is significant at the 10 percent level" (p. 20). Observations for which the h_{ii} is larger then $2p/n$ should be considered to be suspect. Rousseeuw and Leroy (1987) found the hat matrix to be susceptible to masking; they also pointed out that it is based on the classical covariance matrix which is not robust.

Andrews and Pregibon (1978) suggested a linear model which identified deviant or influential observations by deleting observations, calculating the residual sum of squares, calculating the inverse of the inner product matrix formed after deleting observations, and forming a ratio. The Andrews-Pregibon statistic is based on the volume of confidence ellipsoids (Chatterjee & Hadi, 1988) and is a function of leverage and residual (Fung, 1990). Small values of the Andrews-Pregibon statistic are associated with outlying observations. Wood (1983) found that this procedure solves the masking problem, but the number of subsets that need to be examined may be quite large.

Jain (1981) considered five recursive procedures for testing the null hypothesis of n observations in a sample being outliers. The procedures include the extreme studentized deviate (ESD), the studentized range (STR), kurtosis (KUR), the R-statistic (RST), and the JST using the interquartile range of the trimmed sample. The first four procedures were introduced by Rosner (1975, 1977).

Schwager and Margolin (1982) focussed on the identification of outliers in a multivariate normal sample using a mean slippage model. They determined that the best test for outliers is based on Mardia's (1970) multivariate sample kurtosis $b_{2,p}$ which can be used in an initial screening for outliers.

Hoaglin, Mosteller, and Tukey (1983) proposed a statistic based on the fourth-spread, d_f. The fourth spread is the range defined by the upper and the lower fourth. Data points which are smaller than $F_l - 3/2d_f$ or larger than $F_u + 3/2d_f$ are considered outliers.

The Mahalanobis distance is a measure of the distance in factor space (Wood, 1983; Stevens, 1984). It is the most widely used procedure for detection of multivariate outliers.

Comrey (1985) described the Mahalanobis d-squared as a "multivariate generalization of using the standard score and the normal curve to determine the probability that a score of a specified size or larger will be obtained" (p. 275). Rasmussen (1988) also saw the Mahalanobis distance as a multivariate extension of Z. According to Rousseeuw and Leroy (1987), the Mahalanobis distance is a measure of leverage. Cook and Hawkins (in discussion of Rousseeuw and von Zcmeren, 1990) found that the Mahalanobis *D* gives similar results to the methods proposed by Rousseeuw and von Zomeren.

Hawkins, Bradu, and Kass (1984) suggested the median tetrad procedure which is not susceptible to masking and swamping. It involves the use of elemental sets to obtain elemental predicted residuals, a combination of tetrad and elemental slope methods.

The least median of squares and the least trimmed squares are "reliable data analytic tools that may be used to discover regression outliers in ... multivariate situations" (Rousseeuw and Leroy, 1987, p. 16). After fitting the majority of the data, the outliers are the points which lie far away from the robust fit. Portnoy (1988) found that regression quantile diagnostics work as well as the least median of squares and that Cooks's *D* is quicker and not much worse.

Graphical procedures suggested by Rousseeuw and Leroy (1987) include: the residual plot which is useful for detecting outliers: and the standardized LMS residual plotted against the estimated value of y_i which "enables the data analyst to detect bad points in a simple display" (p. 237). Chatterjee and Hadi (1988) also discussed graphical methods, such as the frequency distribution of the residuals, plots of the residuals in time sequence, normal or half-normal probability plots, plots of the residuals versus the fitted values, plots of the

residuals versus X_j, $j = 1, 2, \ldots, k$, added variable plots, components-plus-residuals plots, and augmented partial residual plots. Booth, Alam, Ahkam & Osyk (1989) suggested using principal components analysis consisting of "plots of each data set in the plane of a set's first two principal components" (p. 232).

Hadi (1989b) suggested a procedure for identifying multiple outliers in multivariate data. He proposed ordering the data by a robust distance, dividing the data into subsets, computing distances for the basic subset containing p + 1 observations, re-ordering observations according to the new distances, and repeating these steps until one of three possible stopping points are reached. He concluded that this procedure is simple, inexpensive, and effective with both swamping and masking while successful in the identification of multivariate outliers.

Simonoff (1989) recommended two approaches: first, do a "robust analysis and examine the values which are not in line with the robust fit" or second, "specifically examine the data for unusual values" (p. 1). These approaches deal with univariate data; for multivariate data one needs "an appropriate test statistic and a method of ordering the data" (p. 6). For the test statistic Simonoff recommended using the Mahalanobis D; for ordering the multivariate data he recommended using single linkage clustering to avoid masking. Clustering methods should work well with outliers, "since an outlier (being unusual) should cluster by itself" (p. 7). Hair, Anderson, and Tatham (1987) also recommended clustering, both hierarchical and non-hierarchical, as a means of identifying outliers.

Many of the procedures for detecting multivariate outliers are susceptible to either masking, swamping, or both. Huber (77) discussed the poor performance of some methods

in recognizing outliers if two or more are "bundled together" (p. 3) on the same side of the sample. Masking refers to the problems encountered when the procedure is unable to identify all the outliers (Bradu & Hawkins, 1982; Andrews & Pregibon, 1978). Hadi (a) indicated that masking occurs when an outlying subset goes undetected because of the presence of another subset. Barnett and Lewis (1978) defined masking as the "tendency for the presence of extreme observations not declared as outliers to mask the discordancy of more extreme observations under investigation as outliers" (p. 40). The larger the sample the more masking probably occurs due to the larger number of outliers (Beckman & Cook, 1983).

Swamping is the opposite of masking; instead of declaring too few outliers, the procedure declares more outliers than there actually are (Hawkins, Bradu, & Kass, 1984). Swamping is a phenomenon whereby legitimate observations appear to be outliers; Hadi (1989a) indicated that this occurs "when good observations are incorrectly identified as outliers because of the presence of another, usually remote, subset of observations" (p. 2).

Causes of Outliers

Outliers occur in data for many reasons. Among the most commonly cited reasons are errors in collecting, recording, coding, or entering data, and deviations from the experimental design (Seber, 1984; Douzenis & Rakow, 1987; Chatterjee & Hadi, 1988; Portnoy, 1988); Barnett and Lewis (1978) referred to these as human error and ignorance. These are the outliers which require identification in order to be corrected or rejected. Some outliers occur due to violations of the assumptions; they may indicate the model is not an appropriate one for the data, and they will affect the inferences drawn from the procedures

used. Outliers may be due to the "variability inherent in the data" (Grubbs, 1969, p. 1) as with data f om a "heavy tailed distribution such as Student's *t*" (Hawkins, 1980, p. 1); in this case, the "outliers" are actually valid data points and should not be deleted. Data may actually be from two populations with different distributions, in which case the outliers would be observations not from the basic distribution. These outliers should be rejected or given small weights (Hawkins, 1980).

Treatment of Outliers

After an observation has been identified as an outlier, there remains the question of what to do with that observation. Should it be discarded even if it might be a valid data point? If it is not discarded, then what should be done to prevent it from having a disproportionate effect on the results of the analysis? These questions have been addressed since the 18th century with Bernoulli. Various proposals have been made as to the best course of action. One of the first courses of action is to correct the observation if it is due to an error in recording or coding. If the outlier is not due to a data entry error, there are basically three alternatives: rejection, accommodation, and incorporation. Barnett and Lewis (1978) pointed out the importance of deciding whether the outlier is "important in its own right" or whether it is acting "only as an obstruction" (p. 24). Outliers may also lead the researcher to an understanding of important factors in the data which he had not previously suspected. Beckman and Cook (1983) referred to this possibility as "detecting alternative, rare phenomena" (p. 121); they are among several authors who stress that identifying outliers is more essential than accommodating them.

Summary

Outliers have been called "one of the most vexing and yet widespread of statistical problems" (McCulloch & Meeter, in Beckman & Cook, 1983, p. 152). Many procedures for identifying outliers have been developed. Most of the procedures function in the following ways (Andrews & Pregibon, 1978): They proceed sequentially starting with the most aberrant observation, or they proceed without consideration of the influence the "outlier" may have on the focus of the analysis. If the outlier does not influence the outcome of the analysis, there may be no reason for concern in identifying it.

One of the major problems in identifying outliers is the lack of agreement on an operational definition of an "outlier." Most definitions refer to the outlier as being extreme in some manner. The observation may be extreme or outlying in terms of factor space, in terms of the residual, in terms of its undue influence, or in terms of its leverage; in short, the observation does not appear to be from the same distribution as that of the bulk of the data. In order to satisfy the majority of the researchers who work with outlier identification procedures, an operational definition is a necessity; for if researchers are to be able to accept a procedure or even a small number of procedures for identifying outliers, they must first agree on a definition for "outlier." Once a consensus has been reached on a definition, then researchers can proceed in perfecting outlier identification procedures. An accepted definition may also facilitate the decision as to what to do with outliers after identification. The treatment of outliers is contingent on the type of data being studied. If the data consist of variables pertaining to schools, school systems, or teachers, for example, the outliers

would be those which represent the most effective and the least effective in the data set; in such a case the identification of the outliers might be the main focus of the study.

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